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Fourier Transform Spectroscopy as a Continuous Monitoring Method: A Survey of Applications and Prospects

Entropy Environmentalists, Inc., Research Triangle Park, NC

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FOURIER TRANSFORM SPECTROSCOPY AS A CONTINUOUS MONITORING METHOD: A SURVEY OF APPLICATIONS AND PROSPECTS

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16. ABSTRACT

Several field tests of a Fourier transform infrared (FTIR) spectrometer have been conducted. The results indicate that effective use of this type of instrument in the field of continuous emissions monitoring (CEM) is possible under the proper conditions, and within limits currently imposed by practical experience in this application. Certain tradeoffs are necessary, particularly those pertaining to the physical attributes of the spectroscopic system, the conditioning and content of the samples to be analyzed, and the level of sophistication of the necessarily computerized analysis techniques. Determinations of the proper tradeoffs and subsequent limitations have not yet been determined for all desirable CEM applications, but are the subject of continuing research in the private and public sectors.

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Introduction

The selective absorption of infrared radiation exhibited by most gas phase molecules allows their detection and investigation by a number of spectroscopic methods. Fourier transform infrared (FTIR) spectroscopy is one such method, and is for many applications the simplest and most effective means of simultaneously obtaining quantitative information about a number of constituents in gaseous samples. Although the optical techniques employed are more than a century old, they have only recently become practical due to the availability of relatively inexpensive computers.

The Atmospheric Research and Exposure Assessment Laboratory of the U. S. Environmental Protection Agency and the CEM/Engineering Division of Entropy Environmentalists, Inc. are currently carrying out cooperative field and laboratory evaluations of FTIR systems for CEM applications. These studies, in conjunction with a series of interviews with CEM vendors and other researchers in the field, have indicated a number of practical problems which must still be addressed.

The FTIR spectrometer used in these studies is a Model RFX-30, manufactured by Laser Precision Analytical Inc. of Irvine, California. The system employs an internal infrared source, a refractive scanning interferometer, a modular optical bus system, and a pyroelectric DTGS detector. Two sample chambers, a 22 centimeter single-pass cell and a 22 meter multi-pass White cell, have been used in our laboratory and field studies. Control of the optical system and manipulation of the acquired data are provided by a micro-processor mounted on the optical bench and an external IBM compatible PC.

Test Procedures

Approximately 130 hours of sampling at a commercial hazardous waste incinerator (HWI) burning packaged solid waste and 80 hours at a spreader stoker coal-fired boiler have now been completed.

Stack effluent was normally extracted using a heated stainless steel probe. The majority of the FTIR spectra recorded were of effluent (hereafter referred to as condensed/dried sample) which was passed through two 0°C condensers, a 1 micron filter, and a PermaPure^{R} counter-flow dryer before flowing through the FTIR absorption cell.

Diluted samples of two types were also examined during the tests at the HWI. Such samples were cooled by mixing with dilution air to avoid loss of constituent gases to condensation or solution. In one instance, the exhaust of a TECO Model 200/Model 15 HCl analysis system was dried and diverted to the FTIR absorption cell. The dilution ratio was approximately 35/1, yielding a moisture content of just over 1% before drying. At another time, a TECO 900 dilution system was used to dilute the exhaust of a Bodenseewerk HCl analyzer, and the mixture was dried before flowing through the FTIR cell. The 20/1 dilution ratio proved to be sufficient to prevent damage to the FTIR optics.

Results and Discussion

Detection of Various Molecular Species

Several molecular constituents of the stack effluent, including CO_2, H_2O, CO, CH_4, C_2H_2, and SO_2, were easily identified by a simple visual examination of the FTIR spectra. NO and NO_2 are also present in most of the spectra, but are more difficult to detect because the strongest spectroscopic features fall directly under a water band. HCl is also detectable, although it, too, falls partially under water features, and is not a particularly strong absorber. In addition, several intense but as yet unidentified spectral features exist in at least some of the sample spectra.

To date, all quantitative analyses have been carried out as follows: Reference spectra of NBS traceable calibration gases were recorded in the laboratory, typically at two or three concentration levels per species of interest. Absorption features for each are chosen on the basis of absorption strength and lack of interference with other constituents. The absorbance of a band is an approximately linear function of the concentration for a given species, so a simple linear fit of absorbance peak area to the concentration is performed for each. By integrating the unknown sample spectra over the same frequency intervals and interpolating between points in the reference spectra curves, the concentration of the gases for which references are available can be determined. Software supplied with the spectrometer allowed fairly straightforward implementation of this procedure.

The technique is quite effective for many constituents in the samples, including SO_2, H_2O, C_2H_2, and CH_4. The important species CO presents some particular difficulties, and resists accurate analysis under the linear absorbance vs. concentration model outlined above. Software limitations do not currently allow the use of non-linear fits to the reference spectra peak areas. Until new software is developed or becomes available to us, CO concentrations must be estimated by using a linear model with one data point near the actual concentration, or by the addition of a post facto term quadratic in peak area. These techniques, though crude, yield results in good agreement with independent measurements of the CO concentrations using NDIR and interference filter analyzers.

Accurate quantitative results for HCl, NO_2, and NO await the development of software or sampling techniques to alleviate the severe interference with the H_2O spectrum. Initial attempts have been made by simply subtracting one "zero" spectrum of low NO or HCl concentration from a series of similar spectra. This method yields data of sufficient quality to allow approximate measurements to be made, but is undesirable since the concentration in the "zero" spectrum must be measured independently. More promising is the use of curve-fitting routines to subtract the water spectrum from the data before analysis.

Table I summarizes the preliminary results of the analytical techniques described above.

TABLE I. PRELIMINARY RESULTS

Species	Sampling Technique	Lower Detection Limit (ppm)	Quantification Error[a]
CO_2	all	<1	20%
H_2O	dilution	<1	50%
CO	all	~2	~10%[b]
SO_2	all	~5	~5%[c] (10 ppm min)
CH_4	all	~1	~5% (~2 ppm min)
HCl	dilution	~5[d]	----[e]
NO_2	all	~10	----[e]
C_2H_2	condensed/dried	~5	----[e]

[a] Estimated for 50 ppm; generally lower at concentrations above 50 ppm.
[b] Due to non-linear absorbance effects; see text.
[c] Minimum value currently limited by moisture interference.
[d] Including dilution ratio.
[e] Not available

Comparison of the FTIR Spectrometer and Other CEM Analyzers

In both field tests, several analyzers of various types were in operation during the FTIR sampling time. During the coal-fired boiler test, concentrations of the following criteria pollutants were continuously monitored as they exited the FTIR sample cell: O_2, CO, SO_2, and NO_x. Because the entire sample flow passed through the FTIR cell before being distributed to the other analyzers, the concentrations obtained are directly comparable. Some results for SO_2 appear in Figure 1A, which indicates an average agreement to within 10% between the pulsed-fluorescence analyzer and the linear-model FTIR spectroscopic results. An example of the results for CO are presented in Figure 1B. The agreement here is also quite good, although the FTIR concentrations have been multiplied by a constant factor to correct for non-linearity effects (no quadratic term has been included; this accounts in part for the larger deviations at high CO concentrations). CH_4 concentrations have also been obtained from these data, but are zero at all but a few points.

Comparisons of the FTIR spectrometer results to the values measured by other analyzers during the HWI test are more difficult to make. This is because the samples were passed through the FTIR absorption cell at low rates in order to minimize the potential damage to the cell. Typical residence times of gas-phase molecules in the 10 liter absorption cell were from 5 to 15 minutes. This causes some difficulty since concentrations are yielded by the other analyzers with response times of 30-60 seconds, due to their much smaller active volumes and higher sample flow rates.

The following method of averaging the results from the faster analyzers was adopted. The flow of gas through the cell is not laminar since mixing occurs within its large volume, so the "instantaneous" analyzer values were weighted exponentially, using T, the time necessary to refill the cell, as the characteristic decay time in the exponential. T was estimated from the sample flow rate, and adjusted to give a reasonable match between the decay slopes in the observed FTIR data and the time-averaged

analyzer data. The suitable range of T values was found to be quite broad; for the results shown here, T=10 minutes was used.

At the present time, only those HWI data of particular interest have been thoroughly analyzed and averaged for comparison. An example from July 10, 1989 is shown in Figure 2, which gives the time-averaged CO response from a TECO 48 CO analyzer and the quadratically corrected CO value from the FTIR spectra taken over the same time period. This comparison, for which the CO scaling has been further corrected, does not yield a direct comparison of the CO responses, but was performed as a means of adjusting the value of T in the averaging program. Even considering the liberties taken with the adjustable parameters, the level of agreement indicates the appropriateness of the averaging technique.

Figure 3 shows the CH_4 concentration and time averaged total hydrocarbon (THC) concentration as measured in the condensed sample by a Ratfisch Model 24 FID (flame ionization detector) analyzer. The time period shown is the same as for Figure 2. The THC concentrations have been averaged in the same manner as the CO values of Figure 2, and multiplied by three to take into account the use of propane in the calibration of the Ratfisch analyzer. The data seem to indicate that methane is the major hydrocarbon constituent in this sample, except for some brief periods at the beginning of each spike.

The similar data displayed in Figure 4 are more difficult to interpret because of the greater time spacing of the FTIR spectroscopic data, but may indicate the same sort of behavior. Displayed in this Figure are the THC levels of a hot sample stream, as measured by a JUM FID analyzer, and the methane levels measured with the FTIR spectrometer. Also shown is the difference between the two values, labeled NMHC (Non-Methane Hydrocarbons). These trends are interesting because the CH_4 and NMHC reach their maxima at different times, and since neither of their maxima correspond with those of the CO and THC concentrations, which track together.

System Performance and Reliability

Spectra across the 400 to 4400 cm^{-1} range can be acquired with 2.0 cm^{-1} resolution in about 30 seconds, with a signal-to-noise ratio (S/N) of several several hundred in a 15 second integration time. The spectrometer travels well, requiring approximately two hours for installation, warm-up, and minor optics optimization. However, some precautions must be taken to safeguard the instrument's hydrophilic optical elements during transportation. The system has suffered degradation in performance due to errors in shipping procedures during the first field test. A thorough examination of the optical system by the manufacturer showed no serious loss of optical alignment due to its transportation and extended use under unfavorable field conditions.

The most critical components are the mirrors in the multi-pass cell, which have shown less than 1% total transmission loss in over 200 hours of sampling. The cells' KBr windows, which are hydrophilic and cause optical throughput losses when exposed to moisture, have degraded more rapidly and have been replaced once. However, examination of the damaged windows showed that most of the loss was caused by moisture in the purged optical system itself rather than by moisture in the sample, so this problem may be solved by simply modifying the purging technique.

Some initial reliability problems were experienced, but all were related to computer operation. Aside from problems with the sampling systems, computer "down time" at first outweighed any other source of difficulty in operating the system continuously. Upgrades of software and firmware solved the problem, even though the instrument has been operated at ambient temperatures near the upper limit of the specified operating range. The system has operated more than 90% of the available sampling time, and this figure is expected to increase steadily as further improvements are made in the operating environment.

Samples which were condensed but not dried showed considerably higher moisture content, and are therefore subject to some interference effects which are avoided by use of the dryer. Condensed/dried samples, which are known to contain the original concentrations of criteria pollutants (SO_2, NOx, CO, etc.), were found to be suitable for extended analysis. No damage to the optical system of the FTIR spectrometer was detected even after many hours of continuous sample flow.

Spectrometer Design Considerations

A number of design choices are involved in the construction of FTIR spectrometers, and our field studies indicate that several of these have direct impact on the usefulness of the system for various CEM applications.

Resolution. The resolution of an FTIR spectrometer is usually thought of in terms of the minimum spacing between two spectral features for which those features still appear as separate, distinct entities. The usual operational definition resolution is the full-width-at-half-max (FWHM), in cm^{-1}, of a spectral feature known to narrower than the system resolution. All optical systems possess a limit on the resolution they are capable of providing. In the case of the interferometers used in this application, the resolution is usually limited by the difference in optical path length between the two beams in the interferometer, which is generated by the motion of some optical element. For any particular type of interferometer, increasing the resolution (meaning "increasing the system's capability to resolve adjacent features") demands that some optical element be moved a greater distance. Such an increase in "stroke" always requires an increase in engineering difficulty and system price. An increase in resolution must also be accompanied by an increase in computer capability, since the time necessary for calculations is a step function of the resolution (for fixed bandwidth), and because data storage and handling requirements also increase.

FTIR spectrometers are commercially available with resolutions from 16 cm^{-1} down to nearly 0.001 cm^{-1}. The optimum resolution depends on the exact application. For monitoring samples at ambient pressures, it is unnecessary to obtain spectra at resolutions below 0.1 cm^{-1} , since the actual width of the spectral features themselves is never less than 0.2 cm^{-1} in such samples. Experienced researchers in the field consider the optimum resolution for this application (taking into account many factors not discussed here) to be approximately 0.5 cm^{-1}. However, systems with lower resolution, in the 1 to 4 cm^{-1} range, have also been shown to be quite effective.

Operating Spectral Range. The region most commonly used for quantitative spectroscopic applications is the mid-infrared (mid-IR),

extending from approximately 400 to 4000 cm^{-1}. Most commercial FTIR systems are designed for operation in this range. Although some molecules (notably N_2 and O_2) are infrared-inactive and exhibit no absorption in the infrared, the mid-IR is suitable for observing the vast majority of interesting species.

In most cases, the operating range of the spectrometer is determined by the optical characteristics of the system, and is usually limited by the transmission band of the beam splitter. Choices between various types of other components, such as the infrared source, cell windows, protective coatings, and detector, must also be made properly for optimum operation in the desired range.

Absorption Cell. In many CEM applications, the proper design and maintenance of those components which actually come into contact with the sample gases prove to be most important to the success of the instrument. The considerations concerning the FTIR absorption cell are even more critical than for analogous elements of other types of analyzers. Not only are the reliability and longevity of the cell are likely to limit these important aspects of the spectrometer as a whole, but the characteristics of the cell will ultimately determine the number and concentrations of the molecular species to be monitored.

This is apparent when one considers the effect of the cell's optical pathlength on the system's sensitivity, while keeping in mind the types of samples likely to be of interest. If we restrict our attention to the case of small absorbance by some isolated molecule, then the absorbance will increase in proportion to the cell pathlength. The minimum detectable concentration and the uncertainty in the measured concentration will scale inversely with the pathlength, if all other parameters remain fixed. These facts seems to indicate that the longer the pathlength, the better the instrument.

However, there are several other important considerations. First, extra pathlength is achieved by placing mirrors within the cell, and forcing the beam to traverse the cell many times. Since the optical loss per pass must be small in order to maintain the beam intensity, the alignment and surface integrity of the mirrors are critical - and there is no alternative but to subject them directly to the sample gas, which may be highly corrosive and at high temperatures. Second, the types of samples likely to be of interest may contain widely varying concentrations of various molecular species, and their spectra will overlap to some extent. This leads to the possibility that some strongly absorbing molecule (e.g., water or carbon dioxide) will absorb a large fraction of the radiation in some wavenumber region containing information about a weakly absorbing species of interest. In this case, increasing the pathlength increases the sensitivity of the system to the weak absorber only marginally. In fact, it is not difficult to obtain pathlengths at which certain molecules, even in modest concentrations, absorb virtually all the infrared radiation over a reasonable fraction of the instrument's operating range. Additional considerations, such as loss of throughput and larger sample volumes associated with long-pathlength cells, must also be taken into account.

Many of these limitations can be overcome by sample conditioning techniques or detector improvements, and for many applications there may be no substitute for long pathlength.

Detector. For those cases in which interferences between spectral features is minimal, the sensitivity limit is ultimately determined by the S/N. At longer wavelengths, S/N is normally determined by the responsivity and quiescent noise level of the detector. The responsivity is determined by the exact mechanism by which the detector functions, and in most cases cannot be greatly enhanced by adjustments in experimental technique. However, the noise power is generally due to thermally determined mechanisms, so that the use of cooled detectors can greatly enhance the sensitivity of a spectroscopic method.

The workhorse in mid-infrared spectroscopy is the DTGS detector, which provides reasonable S/N levels at or near room temperature. No detector can match the DTGS in terms of ease of use, sensitivity, and ruggedness; for applications such as monitoring criteria pollutants at atmospheric pressure, the DTGS detector, in conjunction with a cell of moderate pathlength, easily provides sufficient sensitivity at current emission limits. The MCT detector offers faster response and much lower noise than the DTGS detector, but requires cooling by liquid nitrogen or a closed-cycle helium refrigerator. Superior response and low noise are afforded by various types of bolometer detectors when they are cooled to liquid helium temperatures. However, the added cost and difficulty of operating these detectors is justified only for laboratory work, and their use is usually restricted to far-infrared systems, where low source power presents extreme sensitivity problems.

Interferometer Design. Fourier transform spectroscopy is a strenuous engineering challenge because of the necessity of physically moving at least one optical element. In order to maintain system alignment, the motion must be controlled by a fast servo loop, usually based on a visible-wavelength laser signal which co-propagates through the interferometer with the infrared beam. Because a wide bandwidth of audio signals must be detected, vibration isolation between the interferometer and its surroundings must also be exceptionally good.

The Michelson interferometer employs a mirror which moves along the beam axis in one arm. This system is employed by many manufacturers, and is used almost exclusively in high resolution laboratory instruments. The requirements for CEM applications, namely continuous service with a minimum of maintenance in industrial settings, make the design and construction of vibration-resistant Michelson interferometers quite difficult. Several manufacturers have developed alternatives to the Michelson interferometer in order to maintain better motion control and vibration isolation. One alternative is to slide a refractive wedge into one arm of the interferometer, thereby introducing a path-length difference without moving a mirror. These systems are easier to shield from vibrations, and require fewer alignment adjustments than other types of interferometers. The tradeoff here is that current models of such interferometers do not offer resolutions below about 0.5 cm^{-1}. At least one manufacturer offers a spectrometer based on a torsionally controlled interferometer, in which the optical elements do not execute travel motions. This method allows better resolution than the refractive wedge, as well as excellent vibration isolation, since the overwhelming majority of external interference comes in the form of linear vibrations.

Computer capability. Computer systems which are capable of collecting, processing, and recording the FTIR spectra for basic CEM

applications are no longer prohibitively expensive. Typical storage needs for such a system are on the order of 50 Kbytes per spectrum. Considering the fact that most systems can provide up to several such spectra per minute, data management quickly becomes an issue if all the spectra are to be saved indefinitely. At higher resolution, both the computational and data storage requirements can be severe. Computer power and cost will therefore prove to be an important factor in those applications which demand considerably more spectroscopic information than is available at 0.5 cm^{-1} resolution, such as the speciation of large, structurally similar hydrocarbons.

Challenges in CEM Applications

The above discussion indicates the level of technical difficulty which must be met in FTIR spectroscopy. Most of the remaining problems in CEM applications are specific to field use.

Sampling Techniques. The content of samples extracted from stationary sources varies widely from site to site, and sometimes from moment to moment. Careful consideration of the difficulties to be encountered in a particular application is therefore necessary, and flexibility of the system to allow for changes in the sample should be provided. To protect the rather expensive elements of an FTIR spectrometer from damage from condensation of water and other constituents, and to relieve some potentially serious interference problems, several different measures can be taken.

One approach is to dry the sample gases by cooling, and then to remove the resulting liquid phase before analysis. Field tests and practical experience have proven that many of the criteria pollutants, such as NO, NO_2, SO_2, CO_2, and CO, are not removed from a sample stream when it is cooled to 0° C. This allows monitoring of these species in a virtually dry sample, and guarantees the integrity of the analyzer. This method of sample conditioning also lowers the strength of the water absorption features to reasonable levels, allowing accurate analysis for these pollutants without sophisticated mathematical modeling. Several hydrocarbon species can also be observed in such samples, so for many applications this will be the most practical sampling method.

However, cooling the sample to remove the water is also known to remove several species of interest, notably HCl and NH_3. It is likely that a number of organic species are also lost in this conditioning process. An alternative is to dilute the sample with dry, inert gas, so that the sample temperature remains above the dew points of the analytes. Of course, the sensitivity of the system is reduced by the dilution ratio, and there is no change in the relative absorption strengths of water and the other constituents, so no relief from the water interference is afforded. It may be possible to adequately compensate for these drawbacks by increasing the pathlength of the absorption cell, by using more sensitive detection, or by increasing the sophistication of the computational analysis.

The only apparent method of maintaining the original concentrations of the sample is to maintain its original temperature during extraction and analysis. The use of a heated absorption cell is then mandatory, and the cell must be subjected to the full corrosive effect of the sample. It doubtful that the integrity of a multi-pass cell can be guaranteed under

these conditions. However, long pathlength is not necessarily an advantage for analyzing samples containing large concentrations of strong absorbers, and with other adjustments (sophisticated detectors, long integration times, and careful mathematical analysis) such a technique may prove effective in many applications.

Spectral Analysis Techniques. Several different mathematical methods for analyzing multicomponent samples are now available in software form, and are supplied by both manufacturers and CEM vendors along with the spectroscopic hardware. All such methods measure the absorbance of the species in the sample, usually over small, specific wavenumber regions. Typically, use of the software requires that the user have access to reference spectra of those molecular species of interest, and the analysis program must be tailored to the desired application.

The current versions of most software packages, because of the reasonable demand for "user-friendliness," are lacking in at least one important respect. The mathematical complexity and subsequently complex failure modes of the techniques are often hidden from the user in the attempt to make use of the software more palatable. The user must have access to both complete diagnostic information regarding the mathematical manipulations involved and the expertise to interpret this information. The mathematical methods provide much more information than the concentrations of the analytes, and this information could be used effectively to provide the users with a confidence level associated with the analytical results.

The procurement of proper standard spectra and the correct adaptation of the analysis programs to their particular application are not always simple matters. It may be simple to operate the software packages but very difficult, and perhaps impossible, to obtain correct results and a good statistical measure of their accuracy with the available programs.

Conclusions

The major advantage of FTIR spectroscopy over other monitoring methods is its broad-banded nature. The mid-infrared region, for which most commercially available systems are designed, contains at least one set of absorption features for virtually every molecule. One spectrum covering this region can therefore contain information about a large number of the molecules present in a given sample. While FTIR spectroscopy is no less likely than any other spectroscopic method to suffer from interferences between different molecules, the high degree of overdetermination afforded by its broad-banded nature makes it possible to detect, analyze, and correct for many such interferences. Furthermore, the information in a spectrum can be permanently stored in digital form, allowing the possibility for re-analysis for species not known to be of interest at the time the data were collected.

The wealth of information provided by FTIR spectroscopy comes at a price. Aside from the actual system price in dollars, which is typically several times that of a single-component gas analyzer, the high degree of sophistication of such systems compared to other CEM analyzers is a possible liability. If additional software development and repairs become necessary for a particular application, they make FTIR spectroscopy more costly, at present, than standard CEM systems. Manufacturers and developers have been able to provide hardy, self-sufficient instruments which are capable of

effective service in many circumstances, but the technology is simply too young to have been proven reliable in long-term service at any particular site. Constant progress toward this goal is being made.

Disclaimer

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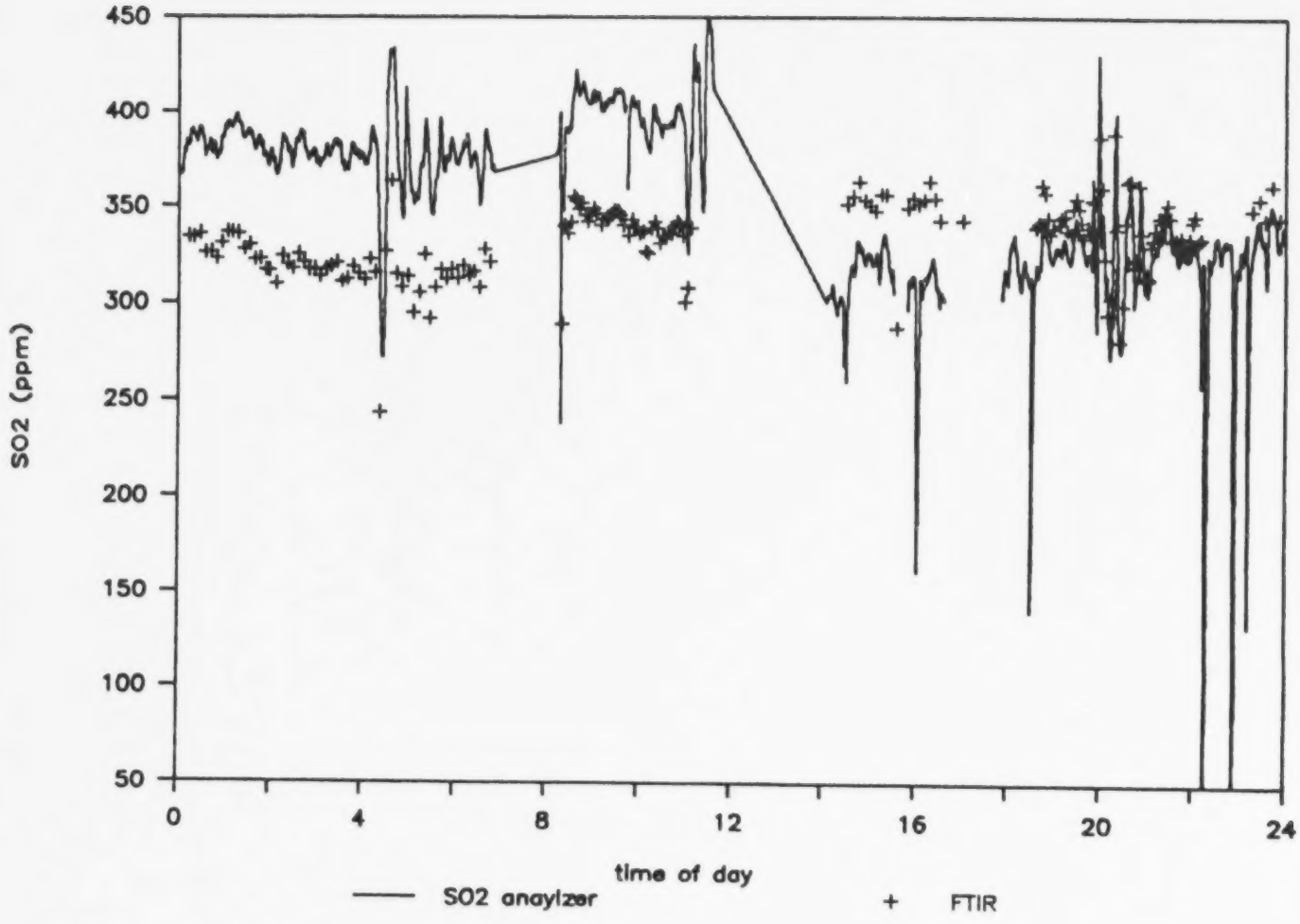

Figure 1A. SO_2 values.

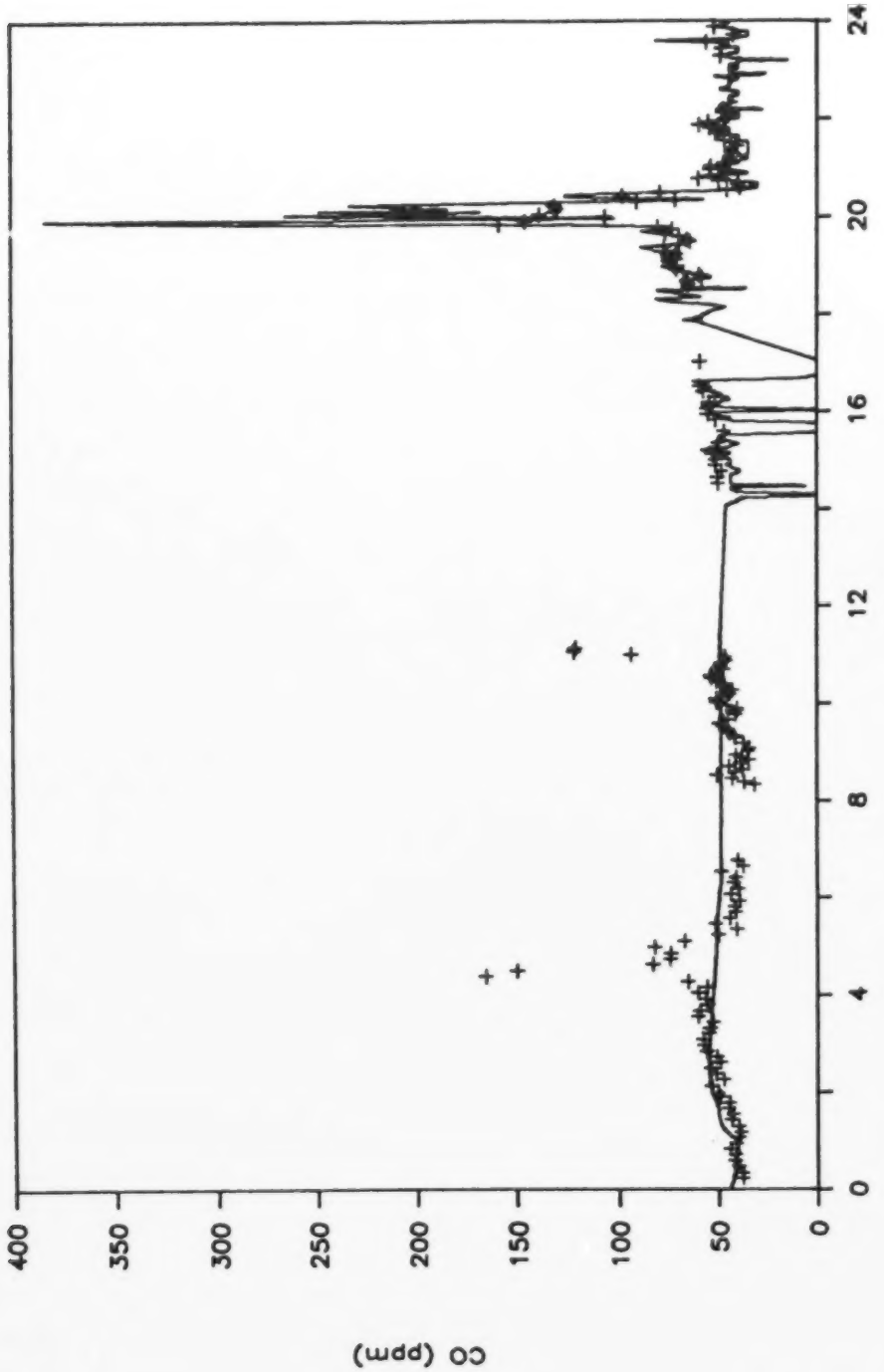

Figure 1B. CO values.

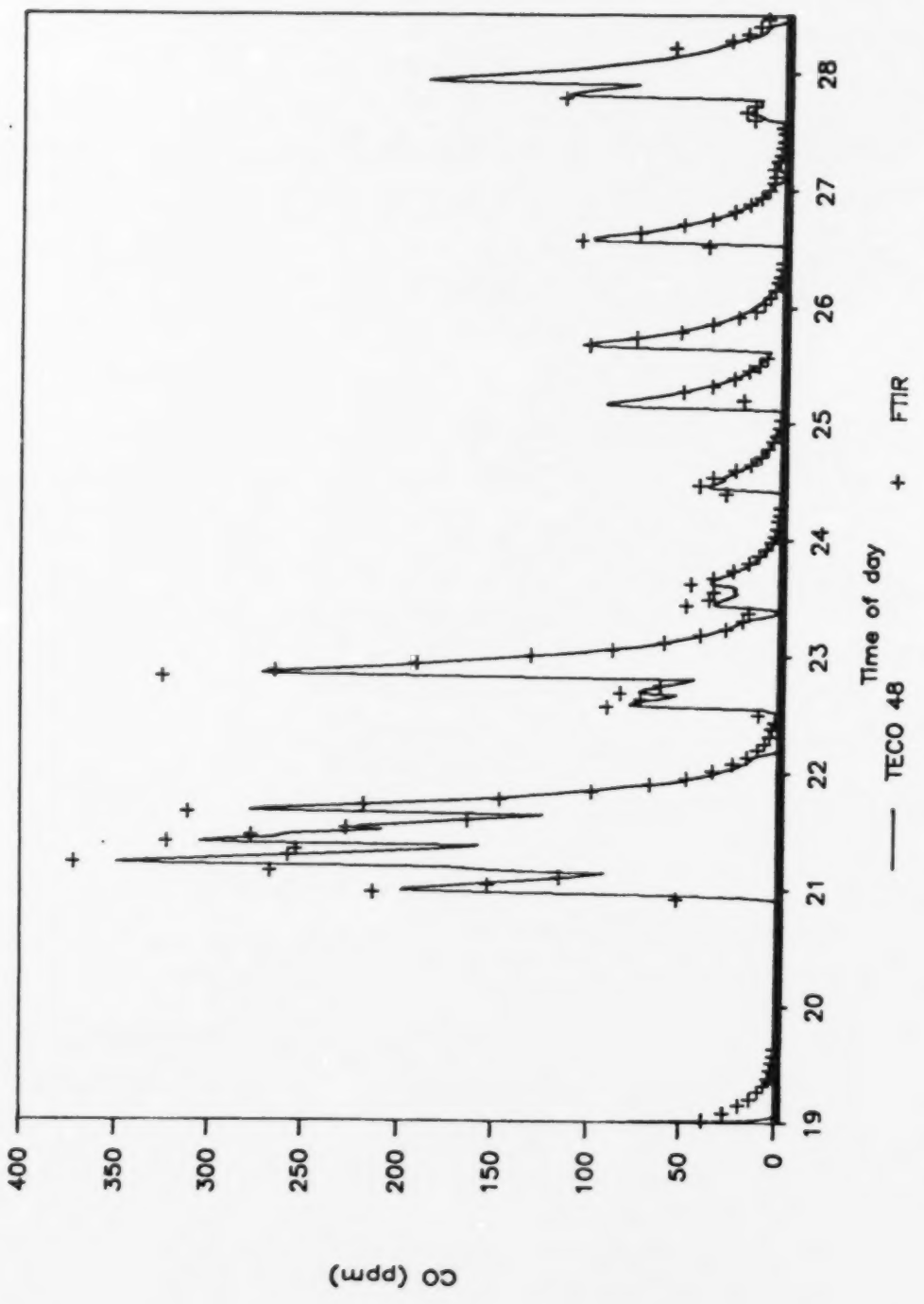

Figure 2. CO comparisons.

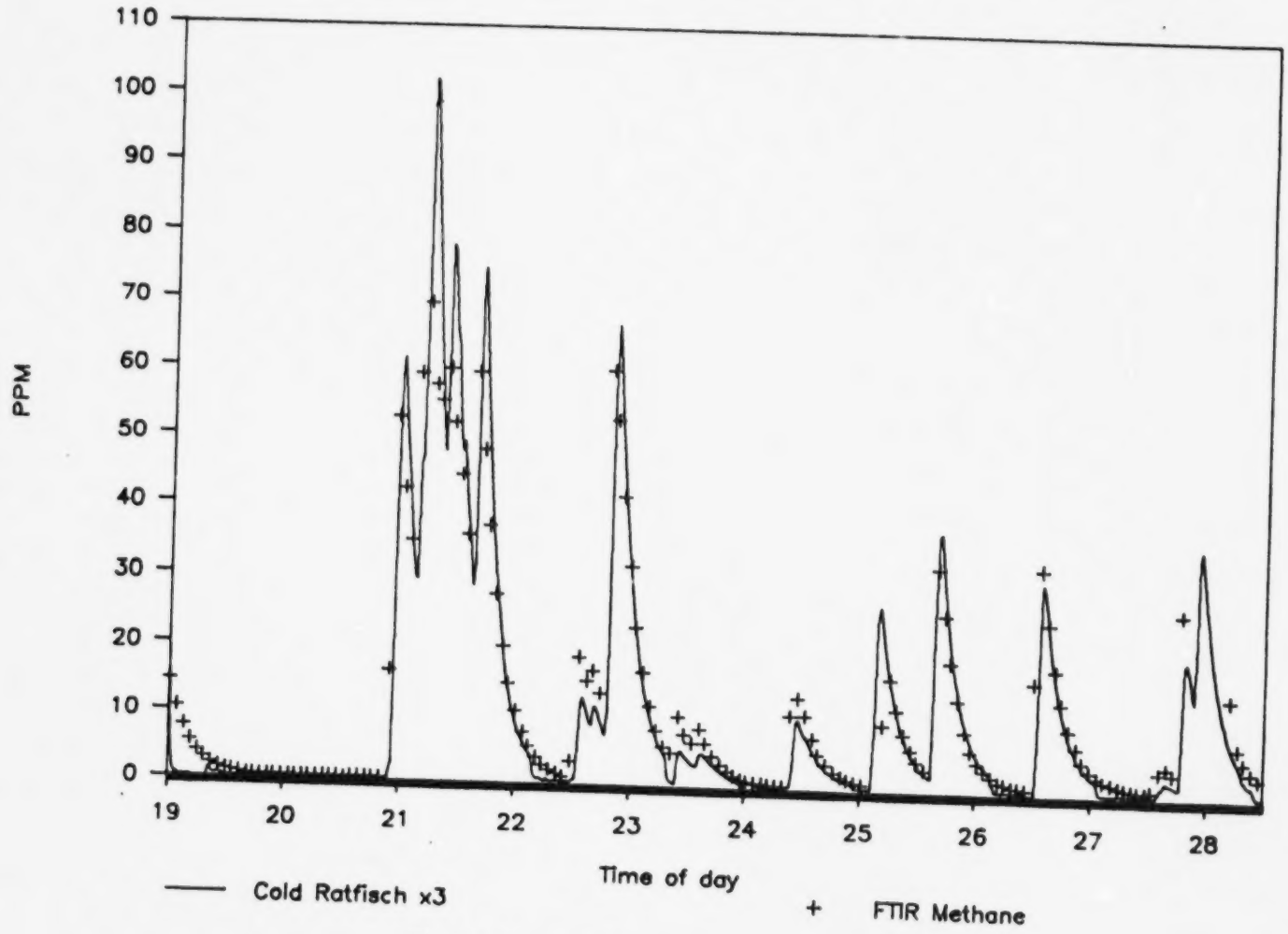

Figure 3. Methane and THC comparisons.

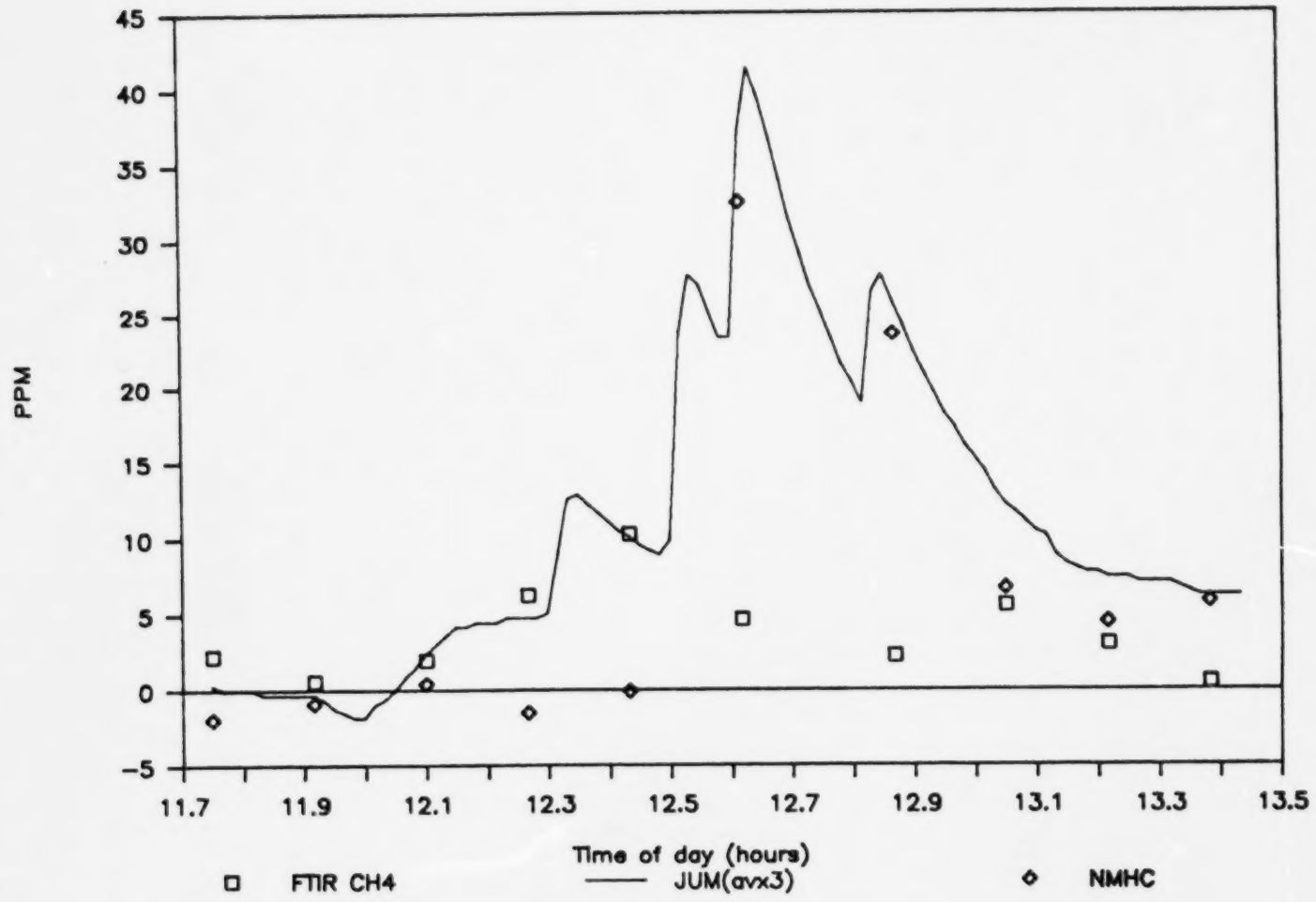

Figure 4. Methane and THC comparisons.

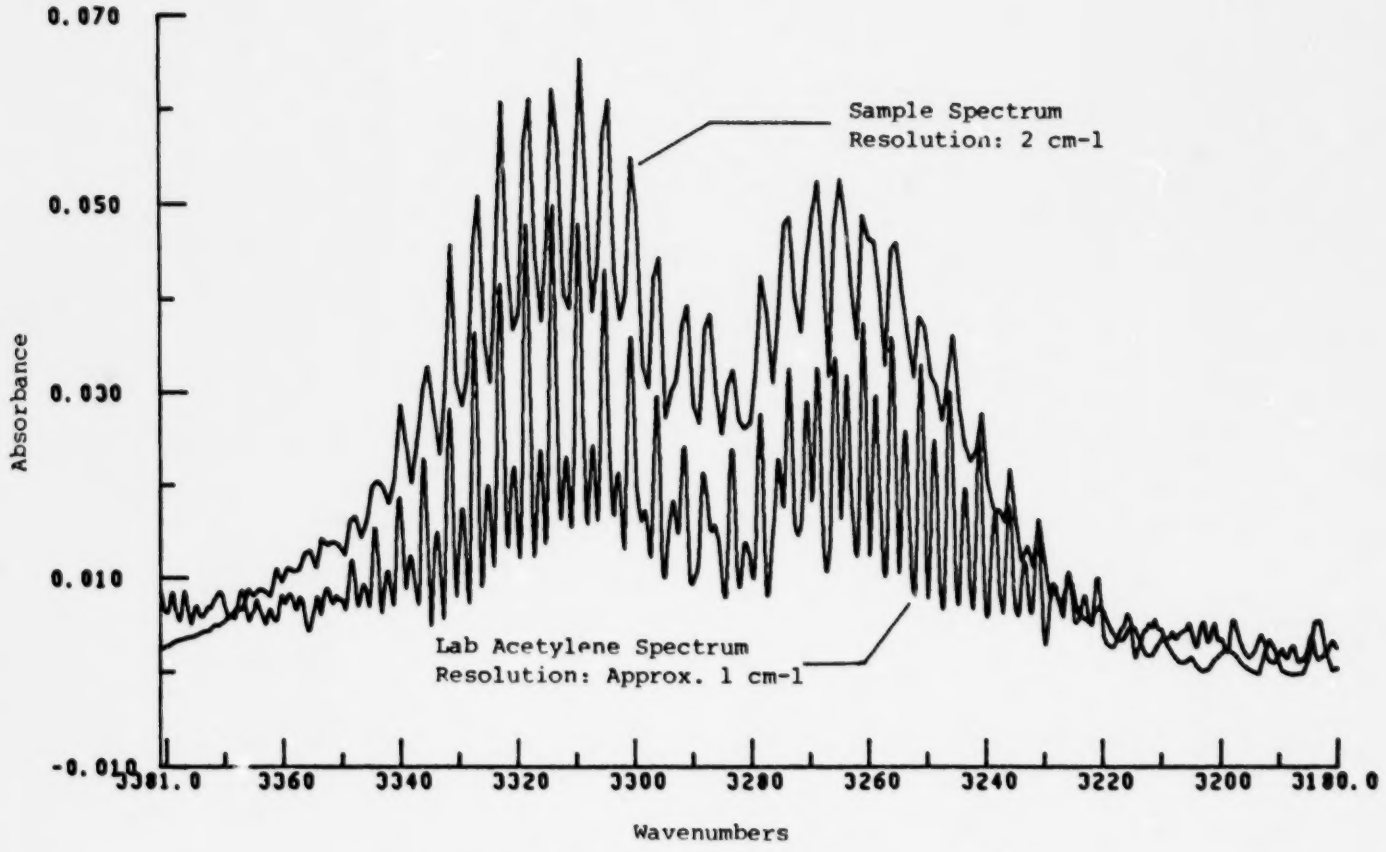

Figure 5. Acetylene Spectra